3.2.5 Rules for Evaluation of Energy Bandgap

In the ATLAS simulator, there are several ways to evaluate the value of energy bandgap for a given material. To uniquely define the approach used, there is a set of rules that are followed in a hierarchical manner. The following is a description of this hierarchy:

1. For each material or material system, there may be a default approach. To determine the default for a given material or material system, refer to the descriptions given in Section 5.4 "Material Dependent Physical Models". If the material system is not listed in this section, then look for default energy bandgap model constants in Appendix B "Material Systems".
2. If you set the EG300 parameter of the MATERIAL statement to a value greater than zero and you do not set the PASSLER parameter of the MODELS statement, the universal energy bandgap model described in Section 3.2.6 "The Universal Energy Bandgap Model" will be used.
3. If you set the EG300 parameter of the MATERIAL statement to a value greater than zero and you set the PASSLER parameter of the MODELS statement, then Passler's model for temperature dependent energy bandgap described in Section 3.2.7 "Passler's Model for Temperature Dependent Bandgap" will be used.
4. If you specify the K.P parameter of the MODELS statement for materials in the InAlGaN system, then the bandgap is taken as the minimum transition energy calculated following the approach given by the strained zincblende tow band model described in Section 3.9.8 "Strained Two-Band Zincblende Model for Gain and Radiative Recombination" or the strained wurtzite 3 band model described in Section 3.9.10 "Strained Wurtzite Three-Band Model for Gain and Radiative Recombination".
5. If you assign the F.BANDCOMP parameter of the MATERIAL statement to a valid filename, the C interpreter function for energy bandgap will be used.
6. If you assign the EG12BOW parameter to a non-zero value, the general terniary bowing model described in Section 3.2.8 "General Ternary Bandgap Model with Bowing" will be used.

3.2.6 The Universal Energy Bandgap Model

The temperature dependence of the bandgap energy is modeled in ATLAS as follows [263]:

$$E_g(T_L) = E_g(0) - \frac{\mathrm{EGALPHA}(T_L^2)}{T_L + \mathrm{EGBETA}} = \mathrm{EG300} + \mathrm{EGALPHA}\left[\frac{300^2}{300 + \mathrm{EGBETA}} - \frac{T_L^2}{T_L + \mathrm{EGBETA}}\right] \quad \text{3-38}$$

You can specify EG300, EGALPHA and EGBETA parameters in the MATERIAL statement (see Table 3-2).

Table 3-2 User-Specifiable Parameters for Equation 3-38

Statement	Parameter	Default	Units
MATERIAL	EG300	1.08	eV
MATERIAL	EGALPHA	4.73×10^{-4}	eV/K
MATERIAL	EGBETA	636	K

Table 3-2 User-Specifiable Parameters for Equation 3-38			
Statement	**Parameter**	**Default**	**Units**
MATERIAL	NC300	2.8×10^{19}	cm^{-3}
MATERIAL	NV300	1.04×10^{19}	cm^{-3}

The default values are material dependent, which can be found in Appendix B "Material Systems". Table 3-2 displays the defaults for Silicon only.

3.2.7 Passler's Model for Temperature Dependent Bandgap

An alternative temperature dependent bandgap model by Passler [204] can be enabled by the PASSLER parameter of the MODELS statement.

The bandgap is given by

$$Eg(T) = Eg(0) - \frac{\mathrm{A.PASSLER} \cdot \mathrm{T.PASSLER}}{2} \left\{ \left[\left(\frac{2 \cdot T}{\mathrm{T.PASSLER}} \right)^{1/\mathrm{P.PASSLER}} + 1 \right]^{\mathrm{P.PASSLER}} - 1 \right\} \quad \text{3-39}$$

where $Eg(T)$ is the lattice temperature dependent bandgap, T is the lattice temperature, A.PASSLER, T.PASSLER and P.PASSLER are user-specified parameters on the MATERIAL statement and Eg(0) is given by

$$Eg(0) = \mathrm{EG300} - \frac{\mathrm{A.PASSLER} \cdot \mathrm{T.PASSLER}}{2} \left\{ \left[\left(\frac{2 \cdot 300}{\mathrm{T.PASSLER}} \right)^{1/\mathrm{P.PASSLER}} + 1 \right]^{\mathrm{P.PASSLER}} - 1 \right\} \quad \text{3-40}$$

where EG300 is a user specified parameter on the MATERIAL statement.

3.2.8 General Ternary Bandgap Model with Bowing

For Ternary compound semiconductors, you can use a bandgap model that continuously and non-linearly interpolates between the bandgaps of the two binary extremes in composition. To enable this model, you must specify the EG12BOW, EG1300 and EG2300 parameters of the MATERIAL statement. EG1300 is the 300K bandgap of the binary compound at a composition fraction of x=0. EG2300 is the 300K bandgap of the binary compound at a composition fraction of x=1. EG12BOW is the bowing factor. The bandgap as a function of composition is given by Equation 3-41.

$$Eg = \mathrm{EG2300}*x + \mathrm{EG1300}*(1-x) - \mathrm{EG12BOW}*x*(1-x) \quad (3\text{-}41)$$

where x is the composition fraction.

You can include the effects of temperature in the Bowing model by specifying the EG1ALPH, EG1BETA, EG2ALPH and EG2BETA parameters of the MATERIAL statement. These parameters are used in Equations 3-53 through 3-55 to calculate the bandgap.

$$Eg_1 = \mathrm{EG1300} + \mathrm{EG1ALPH}\left[\frac{300^2}{300 + \mathrm{EG1BETA}} - \frac{T_L^2}{T_L + \mathrm{EG1BETA}}\right] \quad (3\text{-}42)$$

$$Eg_2 = \mathrm{EG2300} + \mathrm{EG2ALPH}\left[\frac{300^2}{300 + \mathrm{EG2BETA}} - \frac{T_L^2}{T_L + \mathrm{EG2BETA}}\right] \quad (3\text{-}43)$$

$$Eg = Eg_2*x + Eg_1(1-x) - \mathrm{EG12BOW}*x*(1-x) \quad (3\text{-}44)$$

3.2.9 Bandgap Narrowing

In the presence of heavy doping, greater than 10^{18}cm^{-3}, experimental work has shown that the pn product in silicon becomes doping dependent [255]. As the doping level increases, a decrease in the bandgap separation occurs, where the conduction band is lowered by approximately the same amount as the valence band is raised. In ATLAS this is simulated by a spatially varying intrinsic concentration n_{ie} defined according to Equation 3-45.

$$n_{ie}^2 = n_i^2 \exp\left(\frac{\Delta Eg}{kT}\right) \quad (3\text{-}45)$$

Bandgap narrowing effects in ATLAS are enabled by specifying the BGN parameter of the MODELS statement. These effects may be described by an analytic expression relating the variation in bandgap, ΔE_g, to the doping concentration, N. The expression used in ATLAS is from Slotboom and de Graaf [256]:

$$\Delta E_g = \mathrm{BGN.E}\left\{ ln\frac{N}{\mathrm{BGN}\cdot\mathrm{N}} + \left[\left(ln\frac{N}{\mathrm{BGN.N}}\right)^2 + \mathrm{BGN.C}\right]^{\frac{1}{2}}\right\} \quad (3\text{-}46)$$